

Gossonorol

Inchi:	InChI=1S/C15H22O/c1-12(2)6-5-11-15(4,16)14-9-7-13(3)8-10-14/h6-10,16H,5,11H2,1-4H
InchiKey:	WQIRCLDVWQIBLO-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CC(C)=CCCC(C)(O)c1ccc(C)cc1
Mol. weight [g/mol]:	218.33
CAS:	92691-77-5

Physical Properties

Property code	Value	Unit	Source
gf	115.89	kJ/mol	Joback Method
hf	-181.42	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	67.34	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.949		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1625.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2312.00		NIST Webbook
tb	667.25	K	Joback Method
tc	869.10	K	Joback Method
tf	341.95	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.23	J/mol×K	667.25	Joback Method
cpg	556.72	J/mol×K	700.89	Joback Method
cpg	571.27	J/mol×K	734.53	Joback Method
cpg	584.95	J/mol×K	768.18	Joback Method
cpg	597.82	J/mol×K	801.82	Joback Method
cpg	609.95	J/mol×K	835.46	Joback Method
cpg	621.41	J/mol×K	869.10	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92691775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/19-319-7/Gossonorol.pdf>

Generated by Cheméo on 2024-04-20 16:26:18.131863085 +0000 UTC m=+15919627.052440399.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.